High-Throughput Screening Platform for Solid Electrolytes Combining Hierarchical Ion-Transport Prediction Algorithms

Content

1 Main interface

1.1 Components of the main interface

Figure 1 shows the main interface of SPSE. The main interface consists of the following parts:

a) **Navigation bar**: “Home”, “Language switching”, “Search”, “Calculation”, “Upload”, “Sign up” and “Sign in” menus are placed on the navigation bar.

b) **Periodic table**: Click the symbol button to select an element symbol from the periodic table.

c) **Search options**: search options include the space group number, data source, article title, year, BVSE values, data ID, and elements. There is a logical relationship between elements: AND, OR, and NOT.

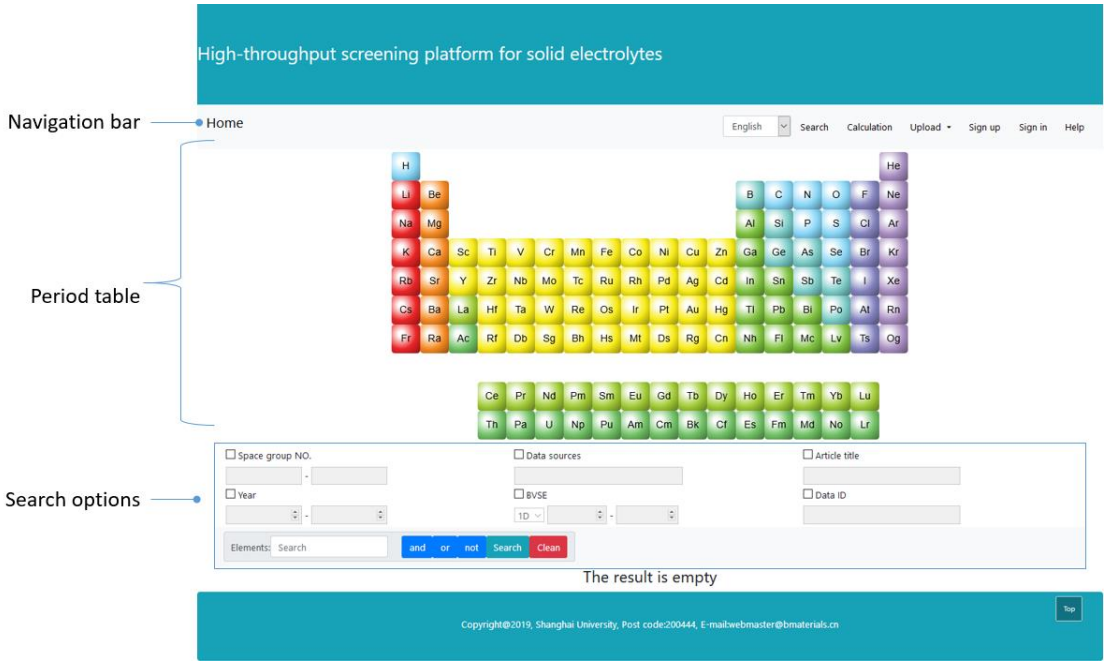


Fig. 1. Main interface-search page

1.2 Menus

a) **Home menu**: Jump to the main interface.

b) **Language switching menu:** Currently, “English” and “Chinese” languages are optional for the website.

c) **Search menu:** Jump to the search interface, also the main interface.

d) **Calculation menu:** Jump to the calculation interface.

e) **Upload menu:**

- Document upload: Jump to the “Document upload” interface.

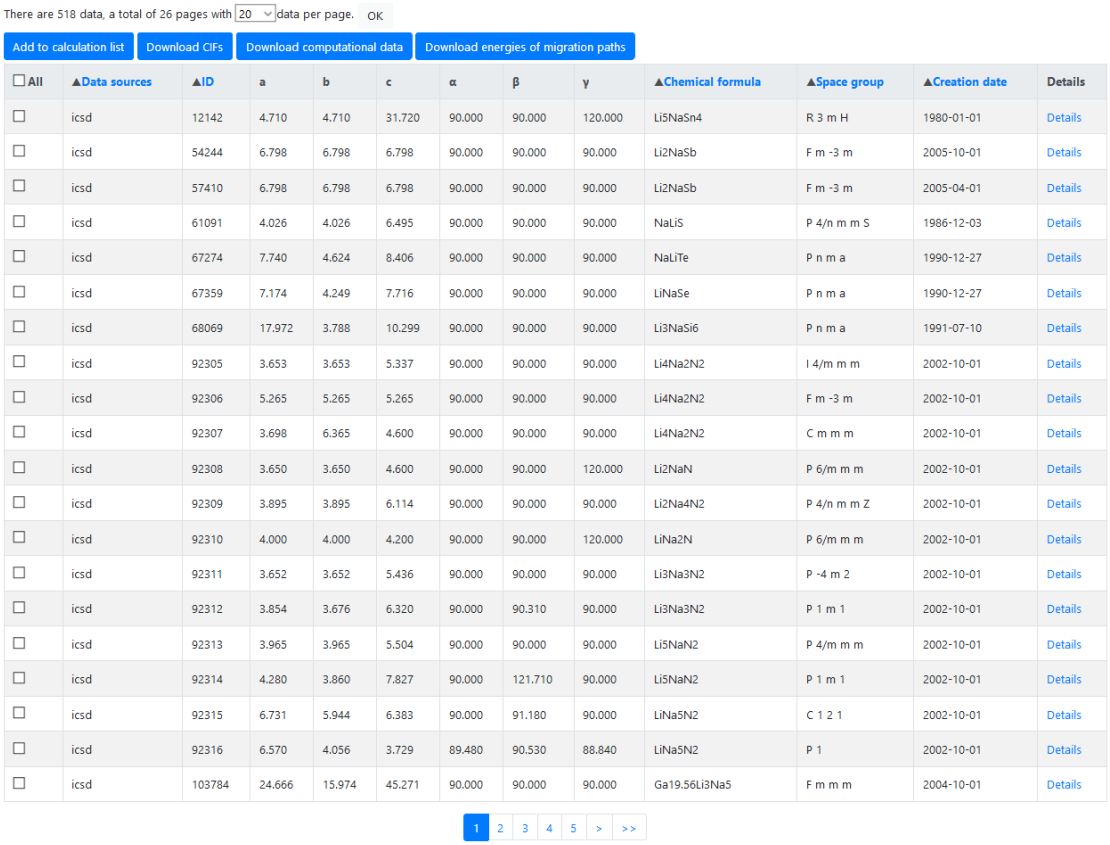
- CIF upload: Jump to the “CIF upload” interface.

f) **Help menu:** Jump to the “Help” interface.

g) **Sign up menu:** Jump to the “Sign up” interface to register a new user.

h) **Sign in menu:** Jump to the “Sign in” interface to sign in.

1.3 Search results


There are 518 data, a total of 26 pages with 20 data per page. OK

Add to calculation list | Download CIFs | Download computational data | Download energies of migration paths

All	▲Data sources	▲ID	a	b	c	α	β	γ	▲Chemical formula	▲Space group	▲Creation date	Details
☐	icsd	12142	4.710	4.710	31.720	90.000	90.000	120.000	Li5NaSn4	R 3 m H	1980-01-01	Details
☐	icsd	54244	6.798	6.798	6.798	90.000	90.000	90.000	Li2NaSb	F m -3 m	2005-10-01	Details
☐	icsd	57410	6.798	6.798	6.798	90.000	90.000	90.000	Li2NaSb	F m -3 m	2005-04-01	Details
☐	icsd	61091	4.026	4.026	6.495	90.000	90.000	90.000	NaLiS	P 4/n m m S	1986-12-03	Details
☐	icsd	67274	7.740	4.624	8.406	90.000	90.000	90.000	NaLiTe	P n m a	1990-12-27	Details
☐	icsd	67359	7.174	4.249	7.716	90.000	90.000	90.000	LiNaSe	P n m a	1990-12-27	Details
☐	icsd	68069	17.972	3.788	10.299	90.000	90.000	90.000	Li3NaSi6	P n m a	1991-07-10	Details
☐	icsd	92305	3.653	3.653	5.337	90.000	90.000	90.000	Li4Na2N2	I 4/m m m	2002-10-01	Details
☐	icsd	92306	5.265	5.265	5.265	90.000	90.000	90.000	Li4Na2N2	F m -3 m	2002-10-01	Details
☐	icsd	92307	3.698	6.365	4.600	90.000	90.000	90.000	Li4Na2N2	C m m m	2002-10-01	Details
☐	icsd	92308	3.650	3.650	4.600	90.000	90.000	120.000	Li2NaN	P 6/m m m	2002-10-01	Details
☐	icsd	92309	3.895	3.895	6.114	90.000	90.000	90.000	Li2Na4N2	P 4/n m m Z	2002-10-01	Details
☐	icsd	92310	4.000	4.000	4.200	90.000	90.000	120.000	LiNa2N	P 6/m m m	2002-10-01	Details
☐	icsd	92311	3.652	3.652	5.436	90.000	90.000	90.000	Li3Na3N2	P -4 m 2	2002-10-01	Details
☐	icsd	92312	3.854	3.676	6.320	90.000	90.310	90.000	Li3Na3N2	P 1 m 1	2002-10-01	Details
☐	icsd	92313	3.965	3.965	5.504	90.000	90.000	90.000	Li5NaN2	P 4/m m m	2002-10-01	Details
☐	icsd	92314	4.280	3.860	7.827	90.000	121.710	90.000	Li5NaN2	P 1 m 1	2002-10-01	Details
☐	icsd	92315	6.731	5.944	6.383	90.000	91.180	90.000	LiNa5N2	C 1 2 1	2002-10-01	Details
☐	icsd	92316	6.570	4.056	3.729	89.480	90.530	88.840	LiNa5N2	P 1	2002-10-01	Details
☐	icsd	103784	24.666	15.974	45.271	90.000	90.000	90.000	Ga19.56Li3Na5	F m m m	2004-10-01	Details

1 2 3 4 5 > >>

Fig. 2. Results of a “Li & Na” search.

For instance, 518 compounds containing Li and Na are obtained by searching for “Li & Na” (Figure 2); by default, 20 data displayed on one page and user can change the amounts. The search results provide common information about the structure, including the data source, data identifier, lattice constant lengths, lattice constant angles, chemical formula, space group, and creation date. More details about the structure can be obtained by clicking “Details” to access the details page. Additionally, data can be downloaded in batches for analysis by clicking the “Download CIFs” or “Download computational data” button. The search page allows users to select the structure(s) of interest and click the “Add to calculation list” button to jump to the Materials Calculation page.

2 Materials calculation interface

The materials calculation interface consists of two parts: calculation list and calculation type. Currently, CAVD, BVSE, ion-transport descriptor, and hierarchical (CAVD + BVSE → NEB) calculations are possible (Figure 3).

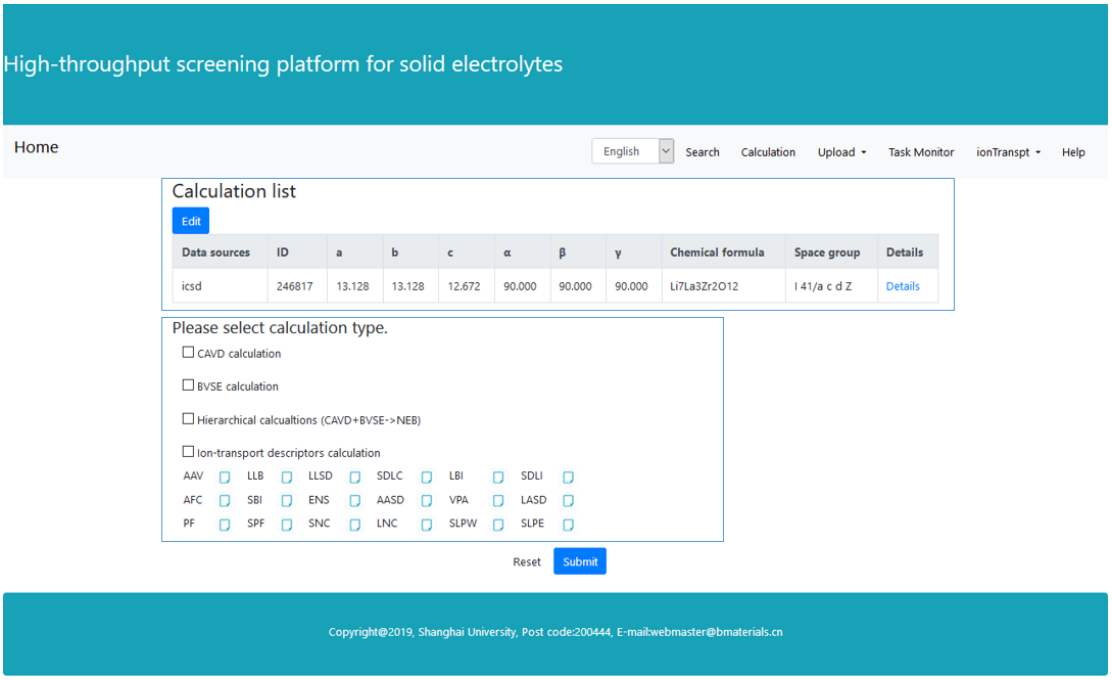


Fig. 3. Materials calculation interface

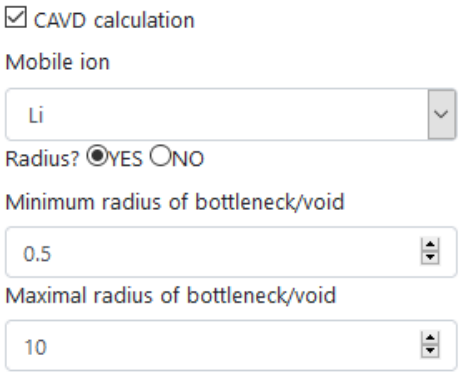


Fig. 4. Parameter setting for CAVD calculation.

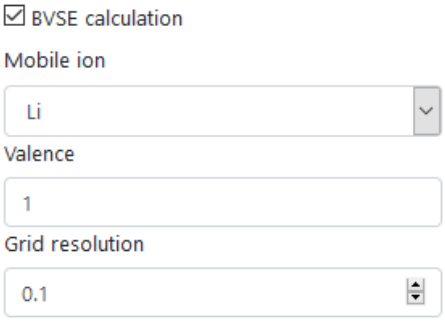


Fig. 5. Parameter setting for BVSE calculation.

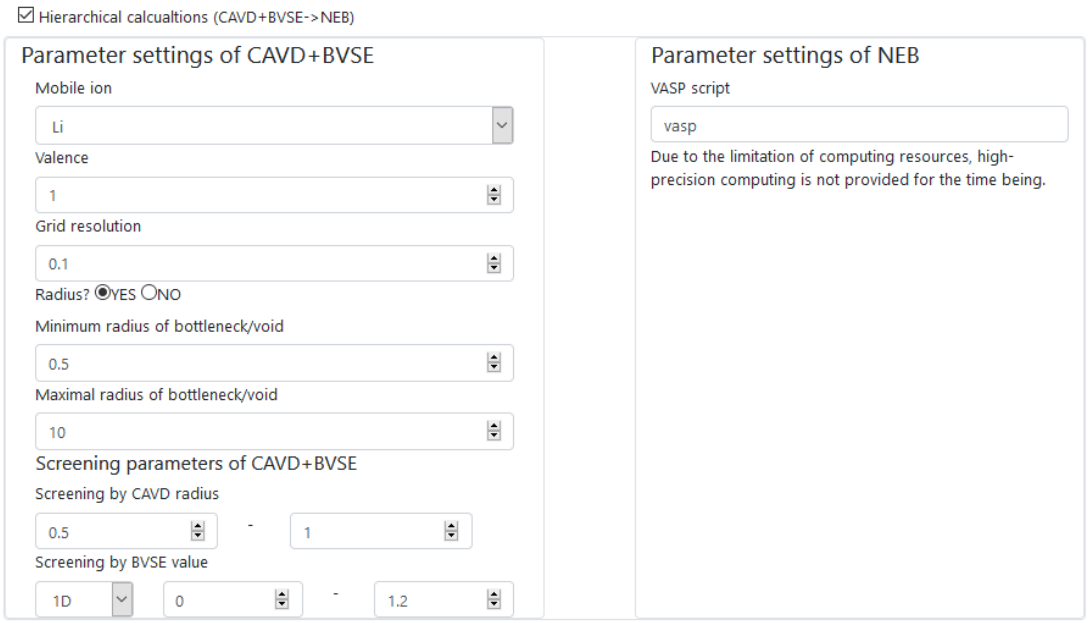


Fig. 6. Parameter setting for hierarchical calculations.

a) Crystal structure analysis by Voronoi decomposition (CAVD): the screening radii of bottlenecks and voids have default values, and the required parameter is the type of mobile ion (Li, Na, Mg, Al, Ag, Zn, Cu, F and O are optional).

b) Bond-valence site energy (BVSE): Similarly, the type and valence of the mobile ion are required for BVSE and hierarchical calculations, and the grid resolution is an optional parameter.

c) Ion-transport descriptor: No parameters are required for the calculation of ion-transport descriptors. The picture " " after the descriptor can be clicked to view the formulas of the 22 ion-transport descriptors.

3 Detail interface

The detail of structure is show in the detail interface. It contain the structure visualization (Figure 7) and structure data.

3.1 Components of structure visualization

a) Tools in the style panel:

- Supercell: View in 2*2*2 supercell, or 10Å box, or reset in unit cell.
- Visulation: View in Ball-and-stick, space-filling, or polyhedra.
- Axis: View along the a, b, or c axis.
- Rotation: Rotation the structure.
- Labels: Lable the atoms in structure.
- Background: View in the black background.

b) Tools in save panel:

Save the CIF file, or state, JPG, PNG or PNG+Jmol.

c) The instructions of JSmol panel are show in Figure 8.

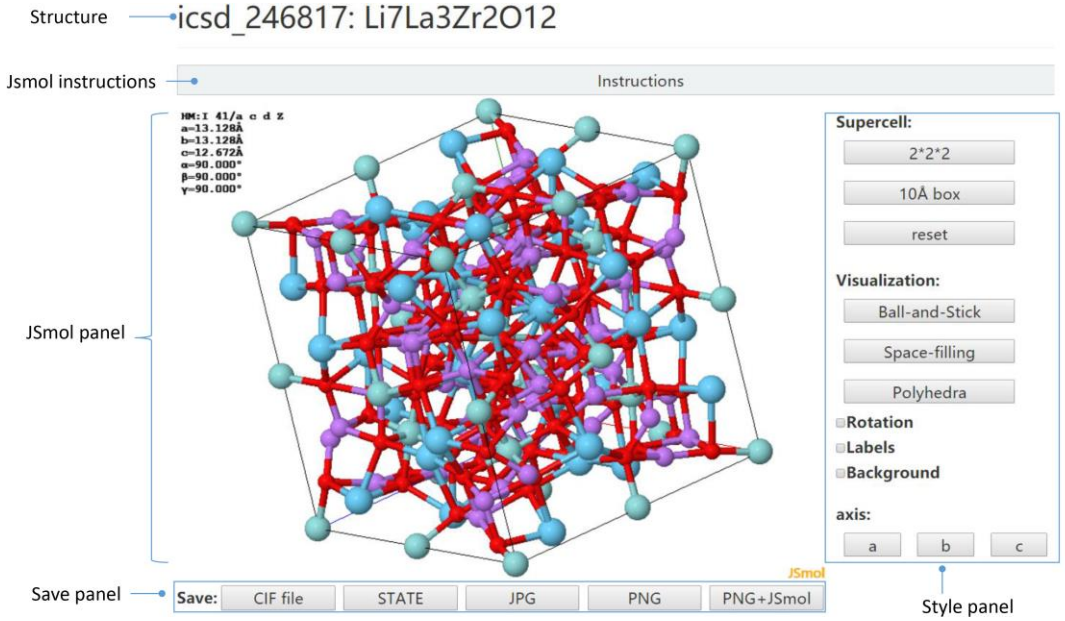


Fig. 7. Structure visualization.

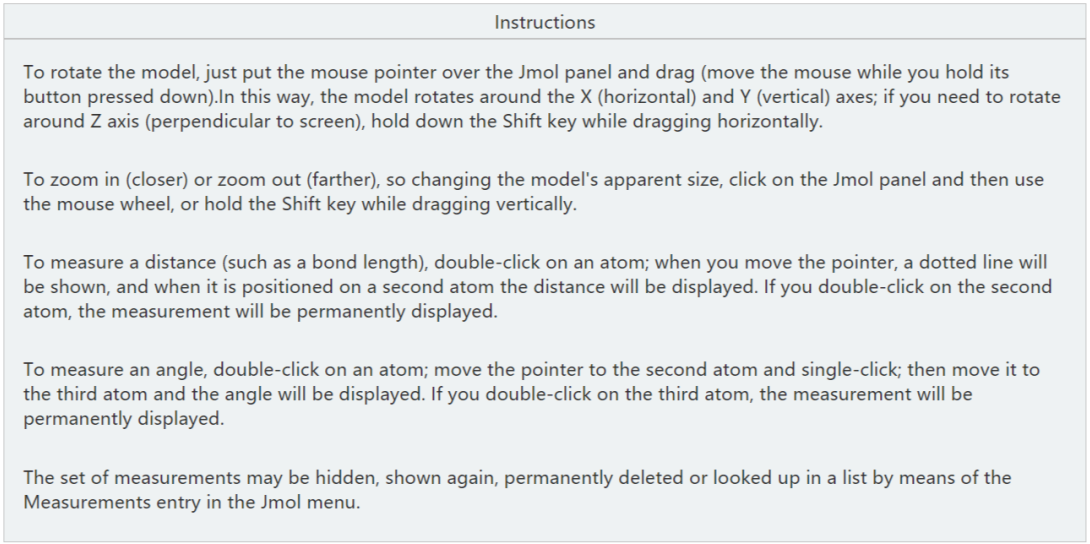


Fig. 8. JSmol instruction.

3.2 Components of structure data

a) structure information (Figure 9)

b) computational data (Figure 10)

- CAVD calculation data;
- BVSE calculation data;
- Ionic migration path;
- Ion-transport descriptor;

Crystal structure

Lattice constant

a	b	c	α	β	γ	volume	z	refine ls r factor all
13.1279	13.1279	12.6715	90.0	90.0	90.0	2183.82	8	0.0076

Chemical formula

Chemical name systematic	Chemical name common	Chemical formula	Chemical formula sum
Lithium Lanthanum Zirconium Oxide (7/3/2/12)	None	Li7La3Zr2O12	La3 Li7 O12 Zr2

Space group

Space group NO.	Space group	Hall	symmetry cell setting
142	I 41/a c d Z	None	None

Valence

Atomic type	Valence
La3+	3
Li1+	1
O2-	-2
Zr4+	4

Atomic sites

Label	Atomic type	Wyckoff	X	Y	Z	Occupancy	Symmetry
La1	La3+	b	0	0.25	0.125	1.0	8
La2	La3+	e	0.127	0	0.25	1.0	16
Zr1	Zr4+	c	0	0	0	1.0	16
Li1	Li1+	a	0	0.25	0.375	1.0	8
Li2	Li1+	f	0.1797	0.4297	0.125	1.0	16
Li3	Li1+	g	0.0806	0.0857	0.8041	1.0	32
O1	O2-	g	-0.0338	0.0548	0.1524	1.0	32
O2	O2-	g	0.0541	0.8529	0.5338	1.0	32
O3	O2-	g	0.1496	0.0276	0.4464	1.0	32

Data sources

Data sources	ID	Article title	Article author
icsd	246817	Synthesis and structure analysis of tetragonal Li7...	Awaka, J.;Kijima, N.;Hayakawa, H.;Akimoto, J.

Date

Creation date	Update date
2010/02/01	2010/02/01

Citations

ID	Year	First page	Last page	Journal volume	ASTM_id	Journal abbrev
primary	2009	2046	2052	182	JSSCBI	Journal of Solid State Chemistry

Fig. 9. Structure information.

Data from calculations or articles

CAVD data

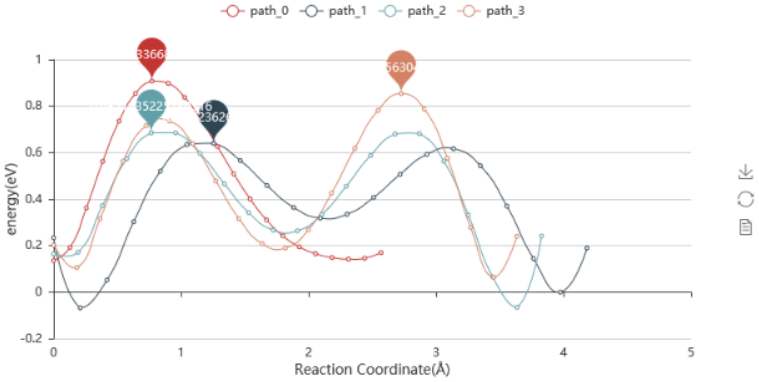
Rf_a	Rf_b	Rf_c	Channel_threshold	con_a	con_b	con_c	Original network	Geometric channel
0.56	0.56	0.56	0.5	True	True	True	.net .VASP	.net .VASP

BVSE data

Mobile ion	BVSE_1d(eV)	BVSE_2d(eV)	BVSE_3d(eV)	BVEL_1d(eV)	BVEL_2d(eV)	BVEL_3d(eV)	GRD file
Li	0.693359375	0.869140625	0.87890625	0.712890625	0.87890625	0.87890625	Download

Ionic migration path

Download the NEB calculation package



Ion-transport descriptors calculation

llb	llsd	sdlc	lbi	sdli	afc	sbi	ens	aasd	vpa	lasd	pf	aav	spf	snc	lnc	slpw	slpe
5.71	2.57	0.89	1.48	1.15	11.0	1.08	2.78	3.18	22.75	1.9	0.83	0.61	11.37	20.71	21.71	0.45	1.54

Fig. 10. Calculation data.

3.3 Download computational data

The BVSE data, CAVD data and ion migration paths can be downloaded in the structure details interface (see Fig. 10). The GRD file and NEB calculation package of $Li_7La_3Zr_2O_{12}$ are downloaded and explained here.

(1) The GRD file is opened with VESTA to visualize migration path. The VESTA settings are shown in Fig 11 and visualization is shown in Fig 12.

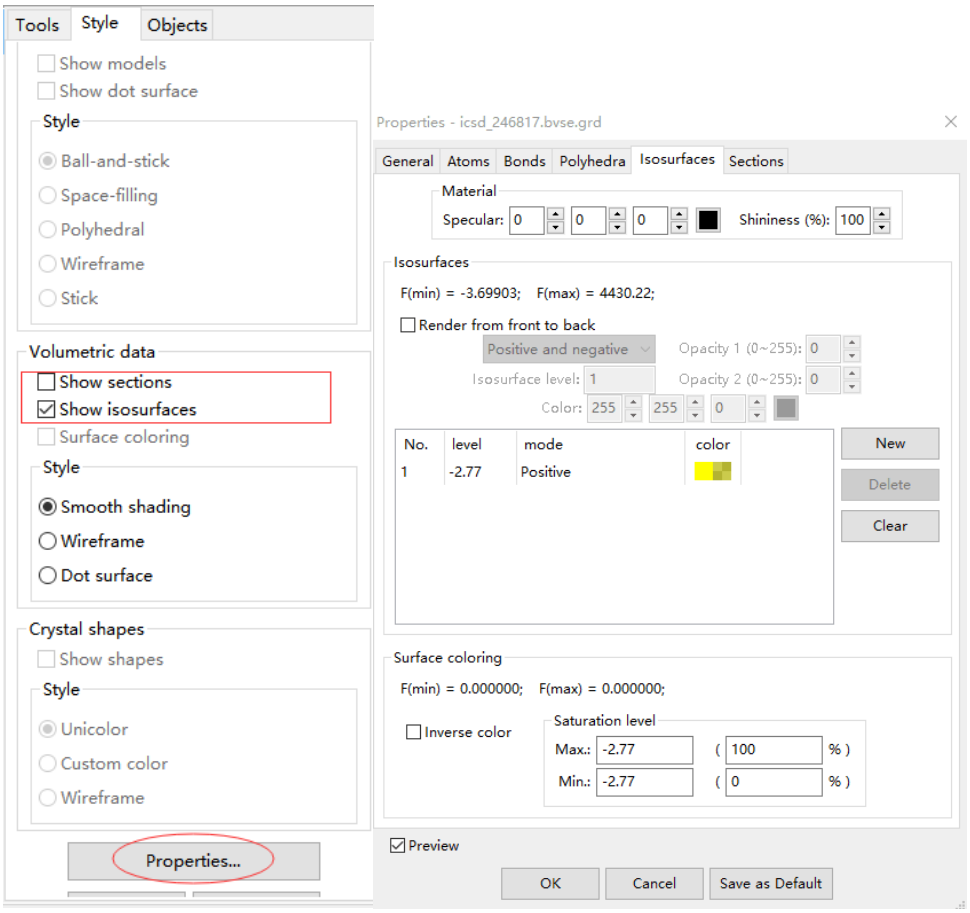


Fig. 11. VESTA settings.

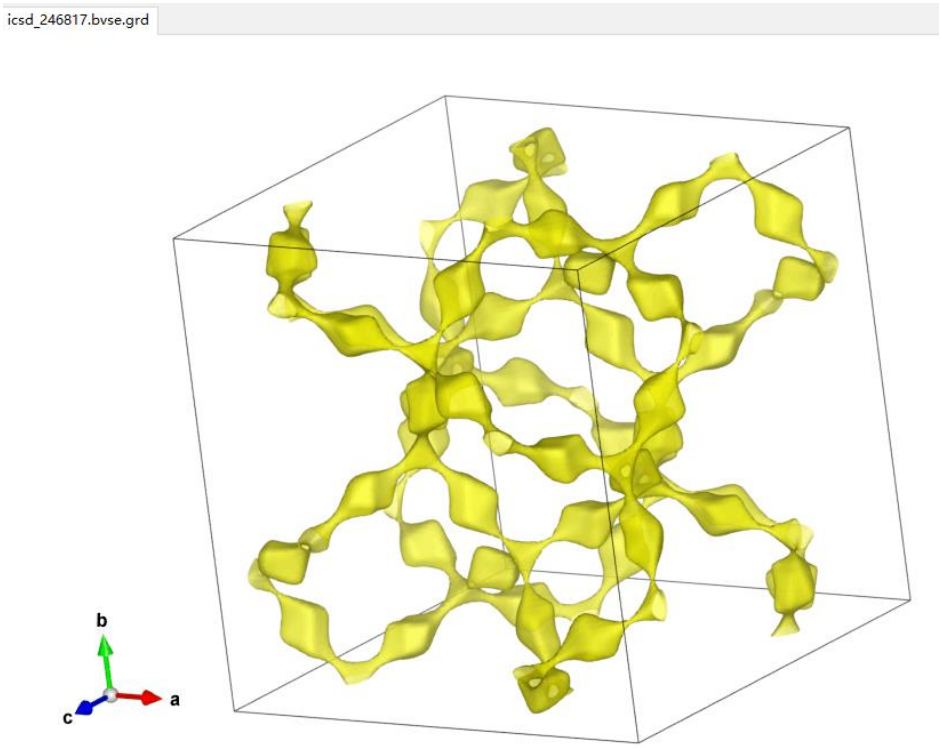


Fig. 12. Migration path of $Li_7La_3Zr_2O_{12}$.

(2) The NEB calculation package is a zip file obtained by hierarchical calculation, which contains all the input files required by NEB VASP calculation of the non-equivalent migration paths in the structure. Taking $Li_7La_3Zr_2O_{12}$ as an example, the NEB calculation data of four non-equivalent paths are included. Among them, INCAR, KPOINTS and POTCAR are input files for VASP to calculate NEB. The decompressed directory is as follows:

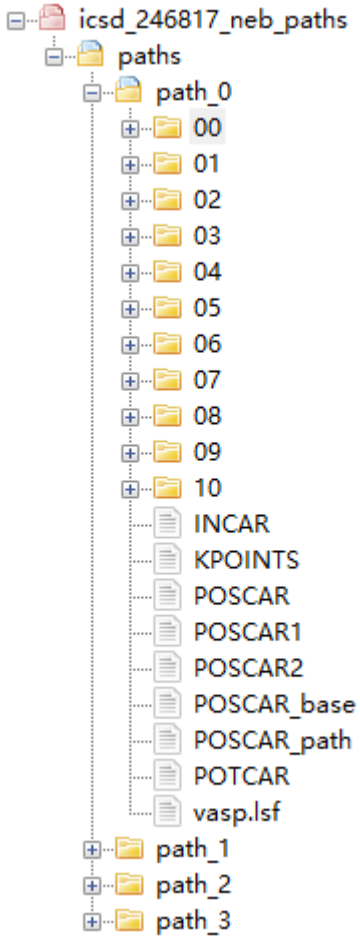


Fig. 13. NEB calculation package.

(3) The POSCAR_path file can be visualized with VESTA:

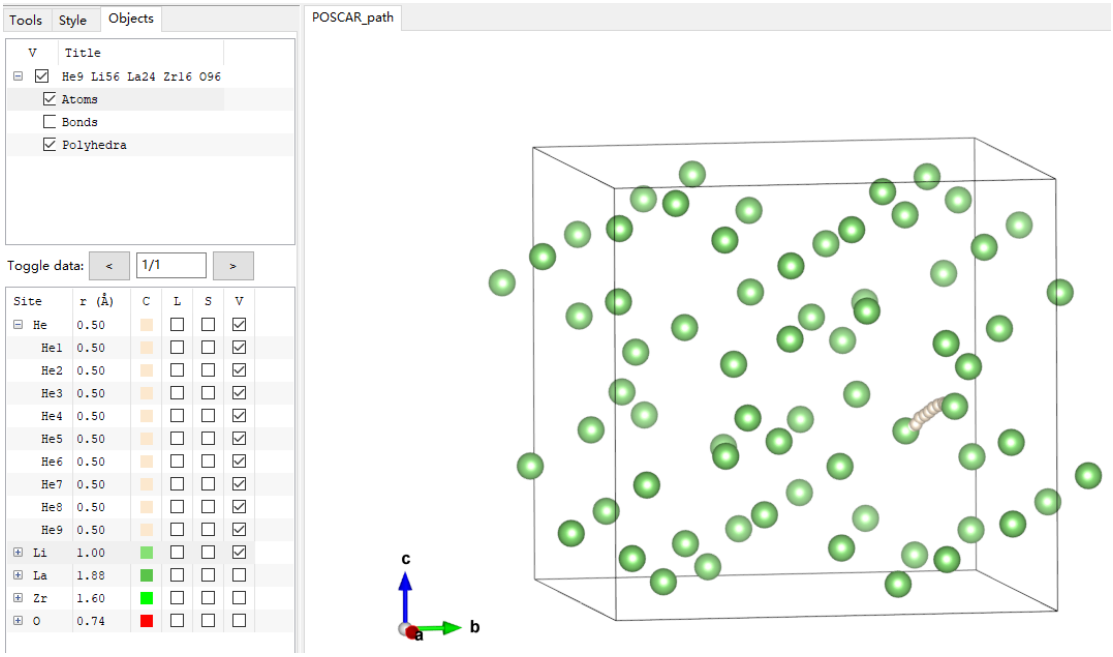


Fig. 14. Visualization of POSCAR_path file.

4 CIF upload interface

In consideration of the demand for additional structures, a Data Upload option is provided for users to upload CIF(s). Users can upload CIF file(s) or .zip file(s) containing CIF files.

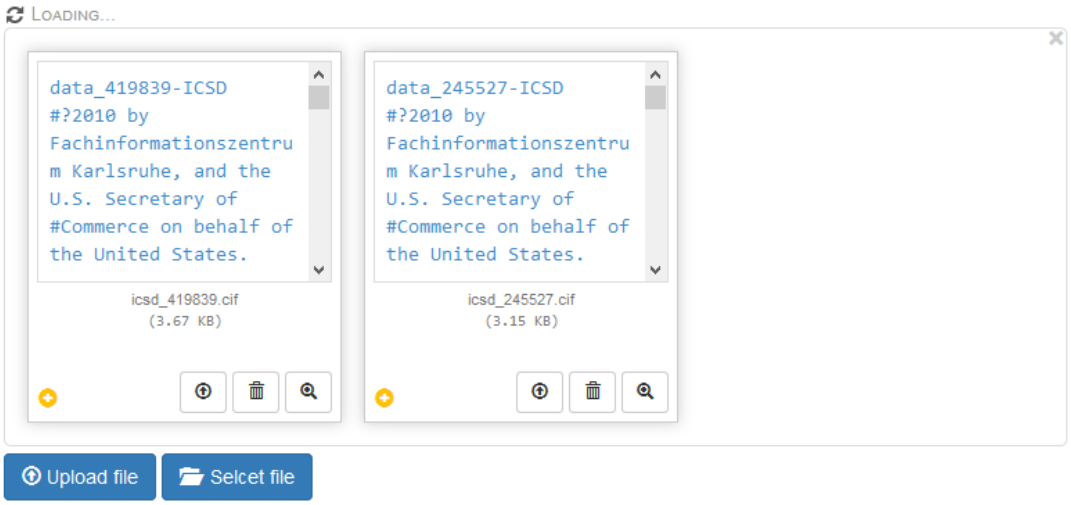


Fig. 15. CIF upload interface.

5 Task monitor

Users can query the states of their submitted tasks using Task Monitor (the states include READY, RUNNING, COMPLETED, FIZZLED, etc.). It shows all tasks submitted by current user. Click “Details” of one task to view the structures of the submission. For each structure, the execution task ID represents the specific task id of the calculation task, and click the id to see the status of current calculation task.

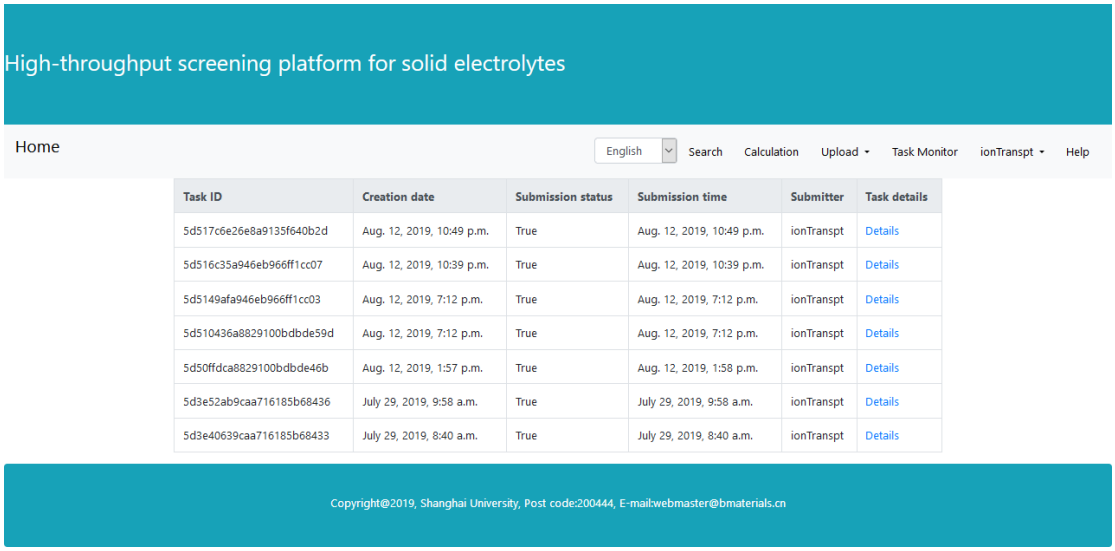


Fig. 16. All tasks.

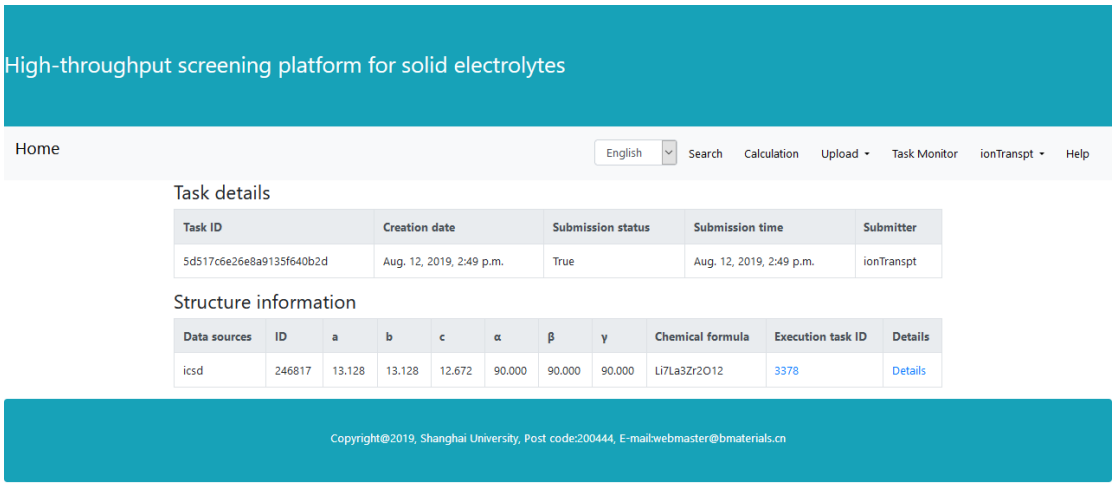


Fig. 17. Task details.

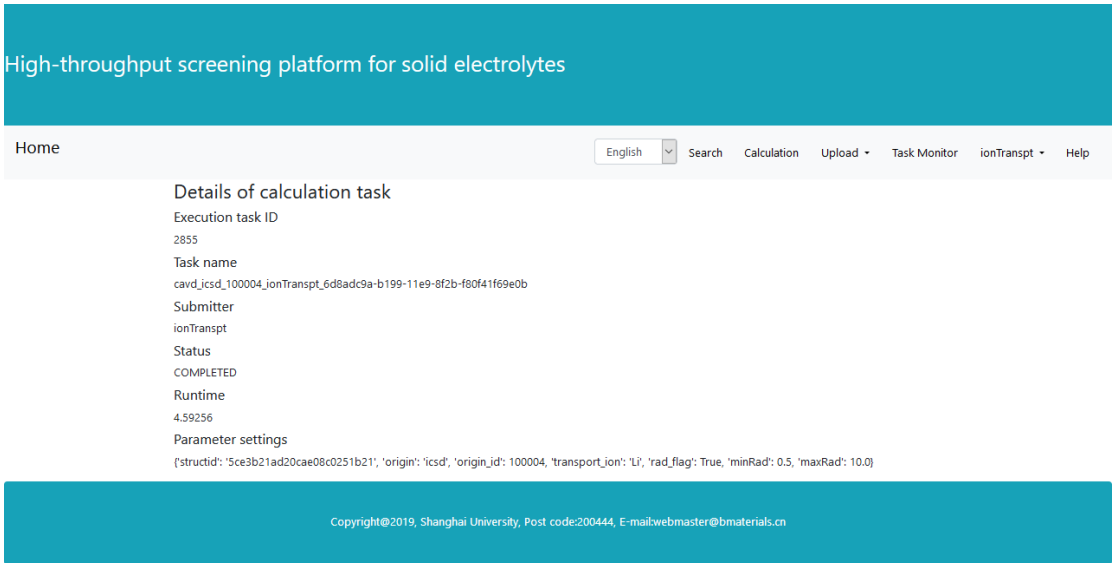


Fig. 18. Details of calculation task.

6 User interface

In order to enjoy complete functions of SPSE, user should sign in the website. If you don't have an account, you can go to the "Sign up" interface to create a new account.

There are five options for users:

a) Sign up;
b) Sign in;
c) Profile;
d) Sign out:
e) Password Reset;
f) Change password;
g) E-mail Addresses.

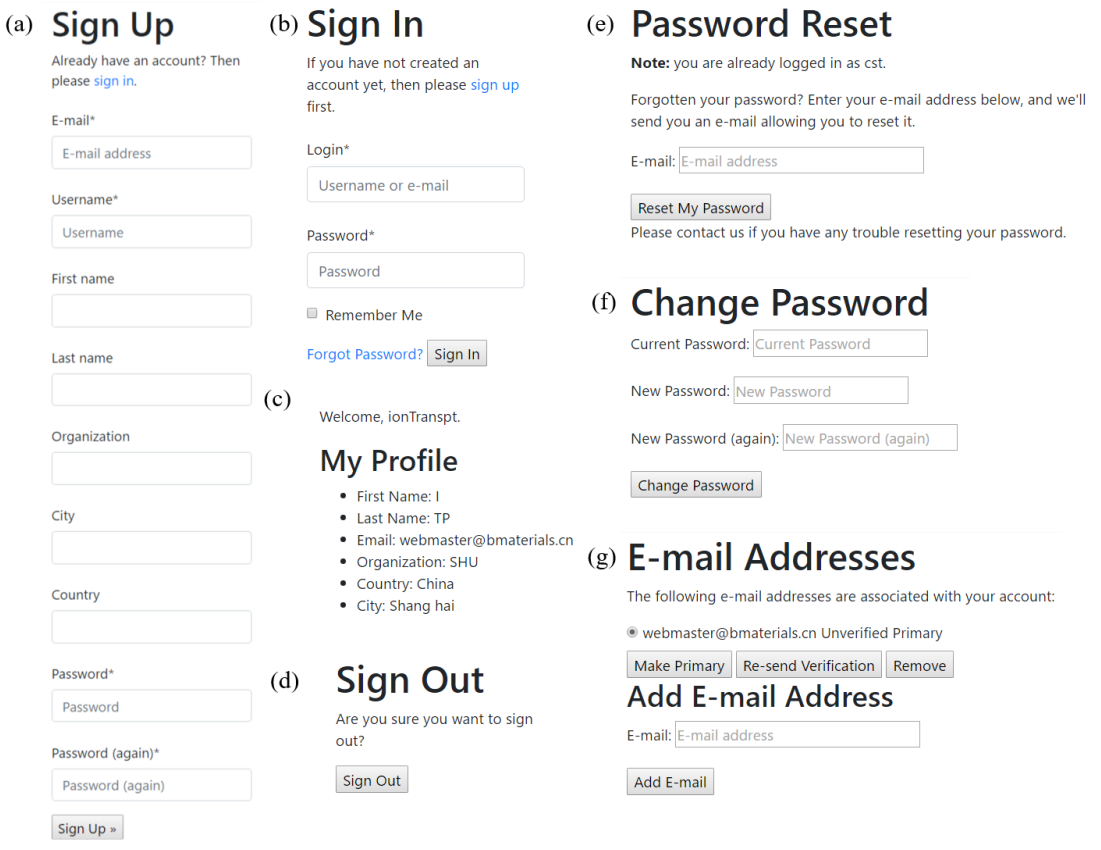


Fig. 19. Sign up interface.

7 Example

7.1 Enter the main interface

a) Click the elements "Li, La, Zr and O" on the period table, and the click the "search" button;

b) Select the structure $Li_7La_3Zr_2O_{12}$(LLZO) whose ID is 246817， and click “add to the calculation list” button;

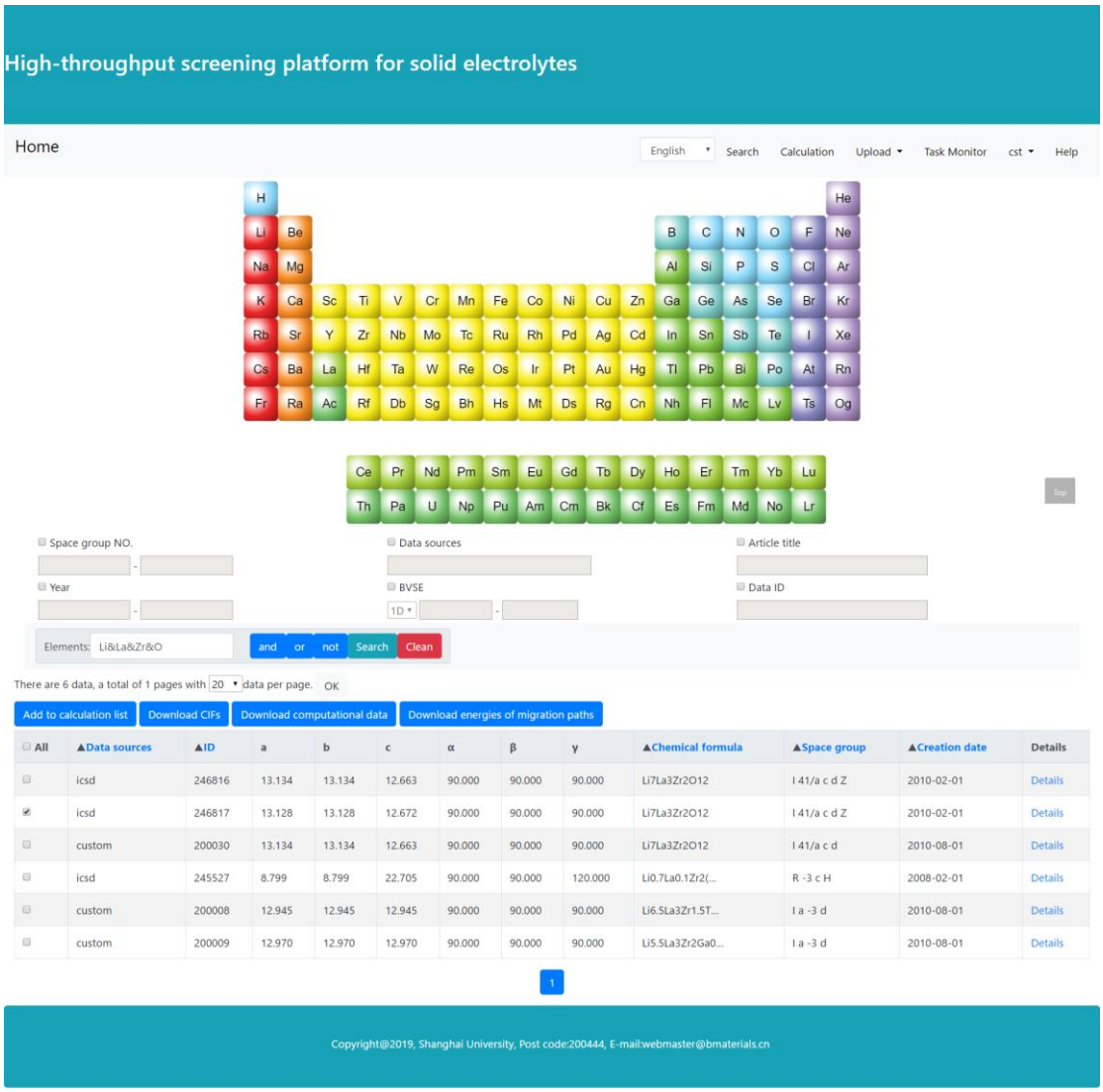


Fig. 20. Select structure and add it into the calculation list.

7.2 Enter the calculation interface

a) Jump to the prompt interface and click the “Calculation” button on the navigation bar;

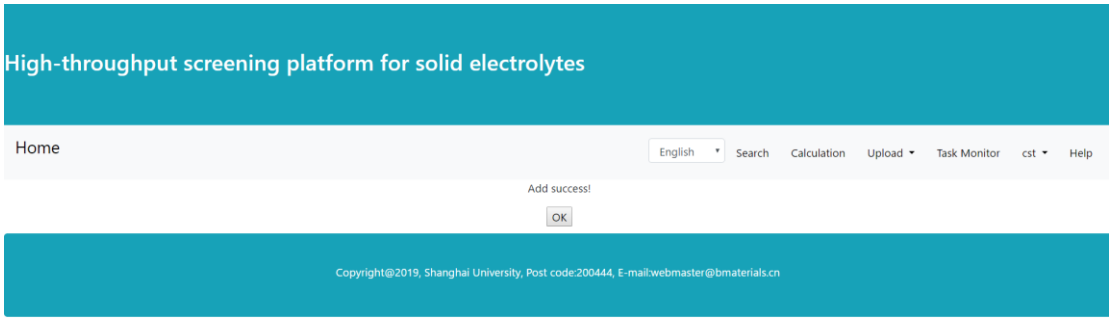


Fig. 21. Add success.

b) Select “CAVD calculation”, “BVSE calculation” and “Hierarchical calculation”. The parameters are default values and click “submit” button.

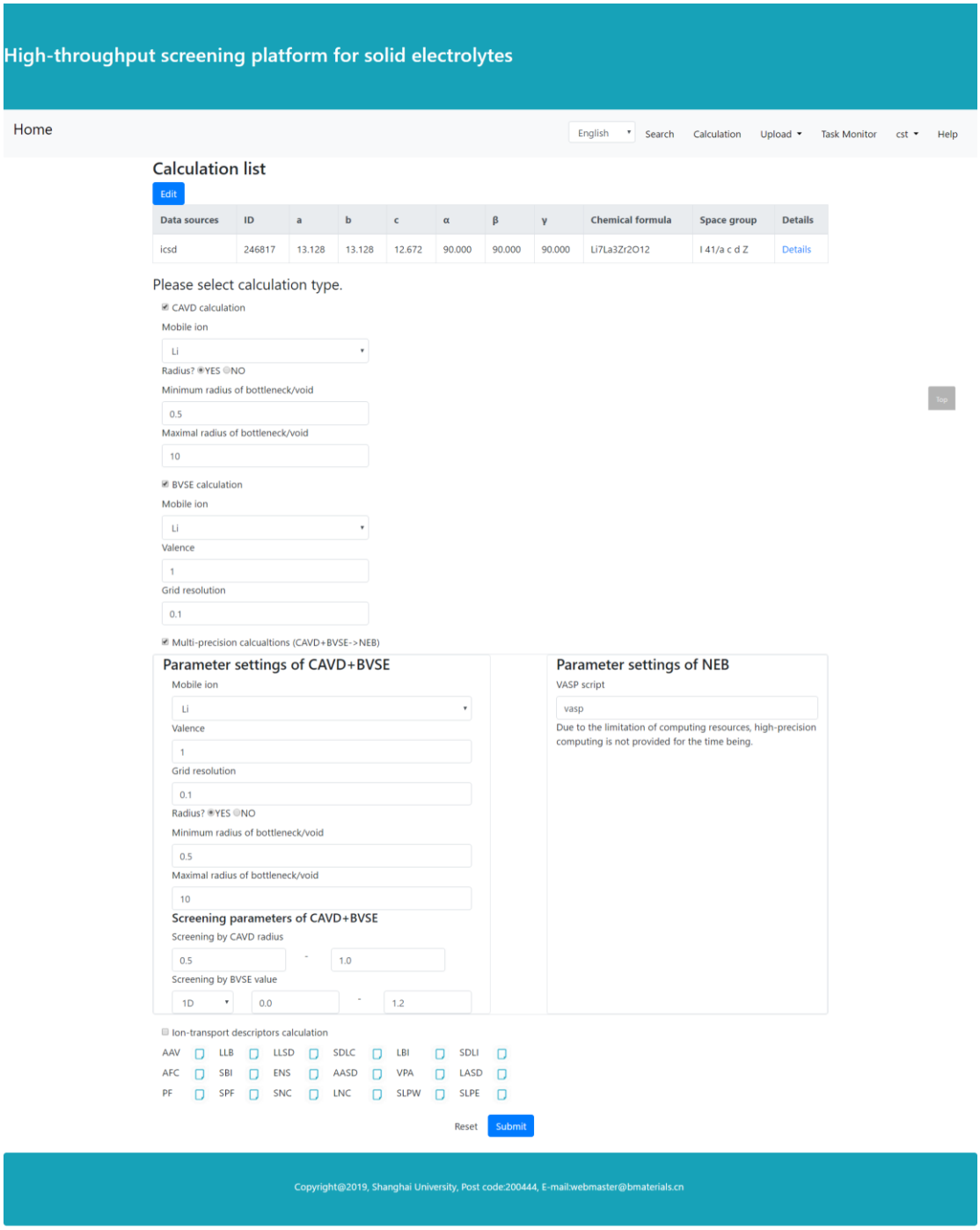


Fig. 22. Calculation interface.

7.3 Enter the “Task monitor” interface

a) Jump to the prompt interface and click the “Task monitor” button on the navigation bar;

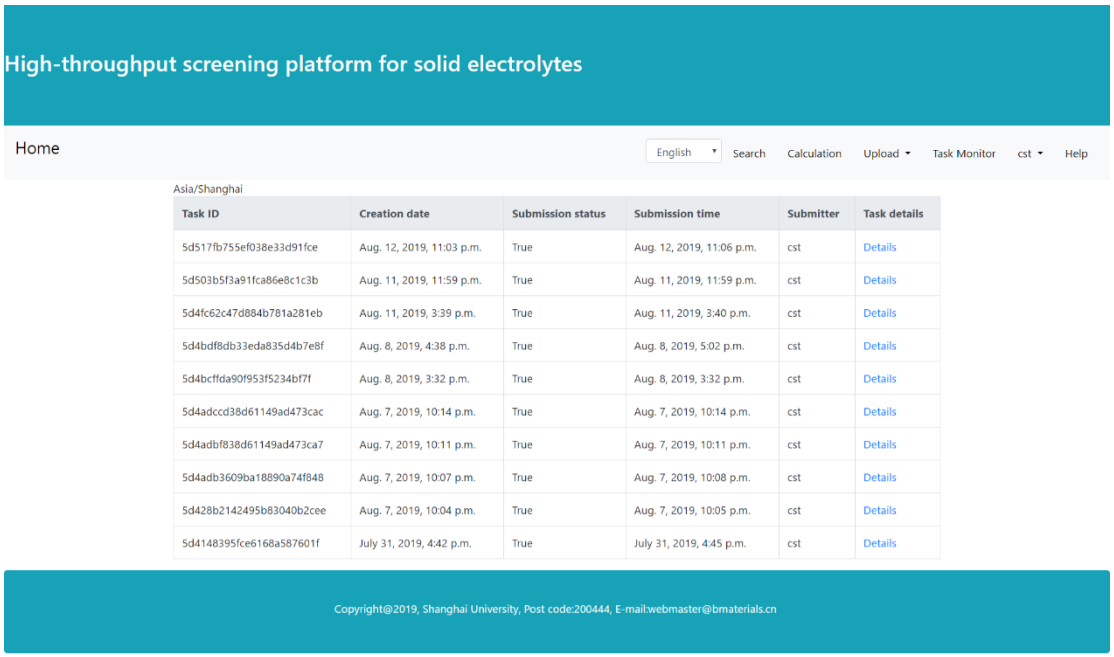


Fig. 23. All tasks.

b) Click the detail of the latest submitted task (such as the submission time is 2019/7/23 00:38)：

c) Click the one of the execution task IDs to view the detail of task.

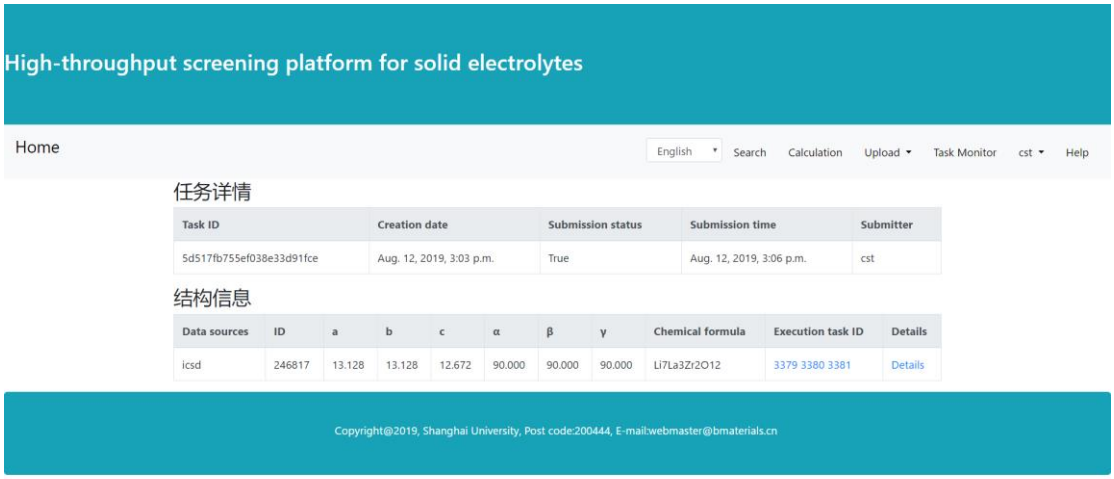


Fig. 24. Task details.

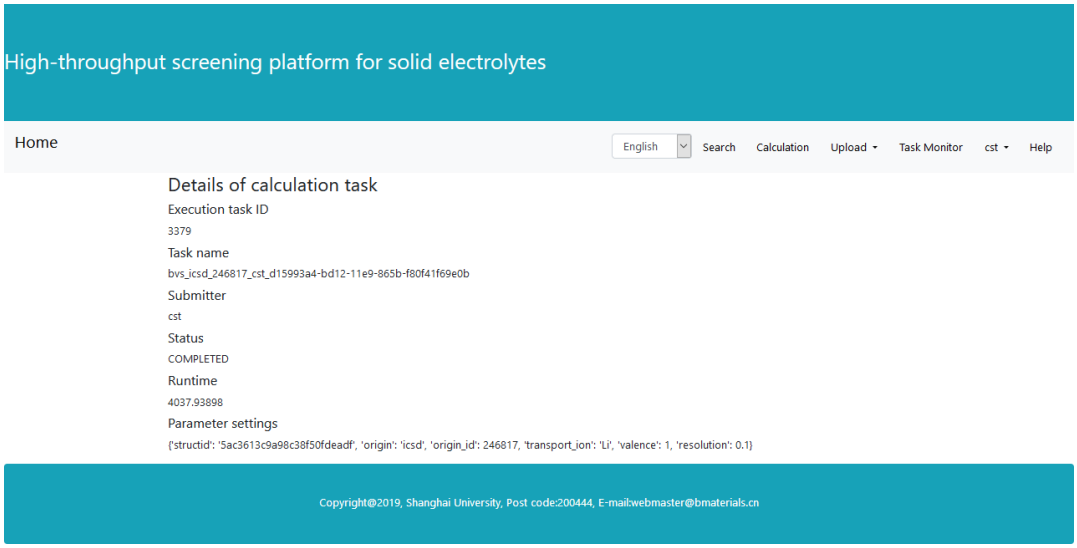


Fig. 25. Details of BVSE calculation task.

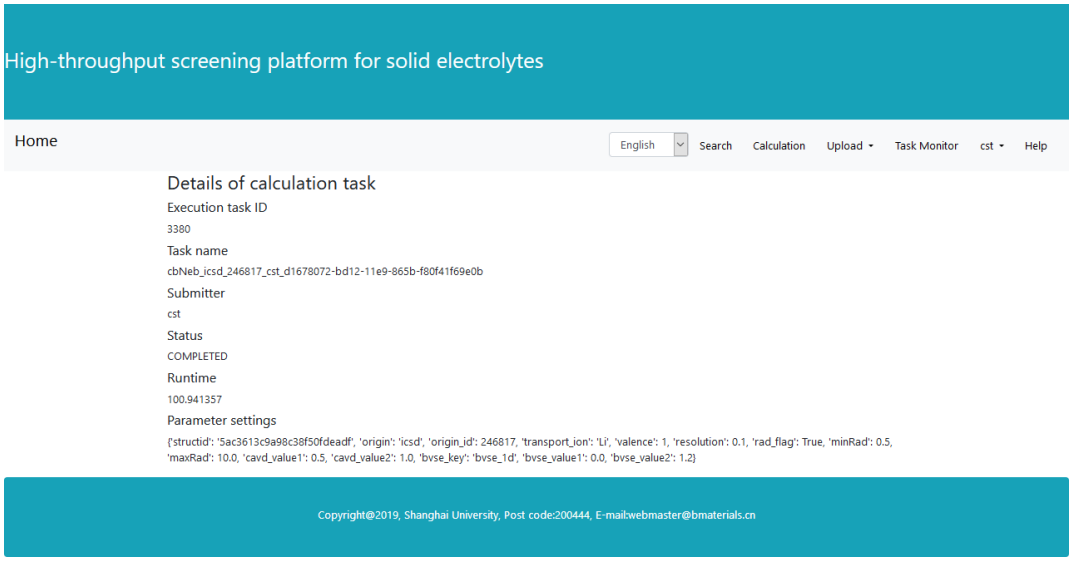


Fig. 26. Details of hierarchical calculation task.

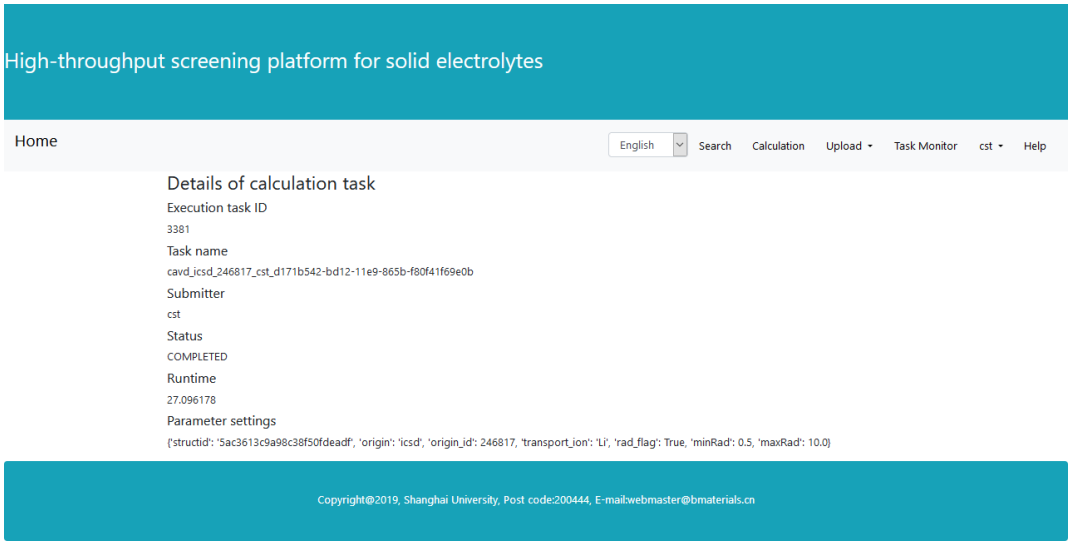


Fig. 27. Details of CAVD calculation task.